

On a relation between the Szeged index and the Wiener index for bipartite graphs

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Abstract

The Wiener index $W(G)$ of a graph G is the sum of the distances between all pairs of vertices in the graph. The Szeged index $Sz(G)$ of a graph G is defined as $Sz(G) = \sum_{e=uv \in E} n_u(e)n_v(e)$ where $n_u(e)$ and $n_v(e)$ are, respectively, the number of vertices of G lying closer to vertex u than to vertex v and the number of vertices of G lying closer to vertex v than to vertex u . Hansen used the computer program AutoGraphiX and made the following conjecture about the Szeged index and the Wiener index for a bipartite connected graph G with $n \geq 4$ vertices and $m \geq n$ edges:

$$Sz(G) - W(G) \geq 4n - 8.$$

Moreover the bound is best possible as shown by the graph composed of a cycle on 4 vertices C_4 and a tree T on $n - 3$ vertices sharing a single vertex. This paper is to give a confirmative proof to this conjecture.

Keywords: Wiener index, Szeged index, bipartite graph.

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1 Introduction

All graphs considered in this paper are finite, undirected and simple. We refer the readers to [2] for terminology and notation. Let G be a connected graph with vertex set V and edge set E . For $u, v \in V$, $d(u, v)$ denotes the *distance* between u and v . The *Wiener index* of G is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V} d(u, v).$$

This topological index has been extensively studied in the mathematical literature; see, e.g., [4, 6]. Let $e = uv$ be an edge of G , and define three sets as follows:

$$N_u(e) = \{w \in V : d(u, w) < d(v, w)\},$$

$$N_v(e) = \{w \in V : d(v, w) < d(u, w)\},$$

$$N_0(e) = \{w \in V : d(u, w) = d(v, w)\}.$$

Thus, $\{N_u(e), N_v(e), N_0(e)\}$ is a partition of the vertices of G respect to e . The number of vertices of $N_u(e)$, $N_v(e)$ and $N_0(e)$ are denoted by $n_u(e)$, $n_v(e)$ and $n_0(e)$, respectively. A long time known property of the Wiener index is the formula [5, 13]:

$$W(G) = \sum_{e=uv \in E} n_u(e)n_v(e),$$

which is applicable for trees. Using the above formula, Gutman [3] introduced a graph invariant, named as the *Szeged index* as an extension of the Wiener index and defined by

$$Sz(G) = \sum_{e=uv \in E} n_u(e)n_v(e).$$

Randić [11] observed that the Szeged index does not take into account the contributions of the vertices at equal distances from the endpoints of an edge, and so he conceived a modified version of the Szeged index which is named as the *revised Szeged index*. The revised Szeged index of a connected graph G is defined as

$$Sz^*(G) = \sum_{e=uv \in E} \left(n_u(e) + \frac{n_0(e)}{2} \right) \left(n_v(e) + \frac{n_0(e)}{2} \right).$$

Some properties and applications of the Szeged index and the revised Szeged index have been reported in [1, 8–10, 14].

In [7], Hansen used the computer programm AutoGraphiX and made the following conjectures:

Conjecture 1.1 *Let G be a bipartite connected graph with $n \geq 4$ vertices and $m \geq n$ edges. Then*

$$Sz(G) - W(G) \geq 4n - 8.$$

Moreover the bound is best possible as shown by the graph composed of a cycle on 4 vertices C_4 and a tree T on $n - 3$ vertices sharing a single vertex.

Conjecture 1.2 *Let G be a bipartite connected graph with $n \geq 4$ vertices and $m \geq n$ edges. Then*

$$Sz^*(G) - W(G) \geq 4n - 8.$$

Moreover the bound is best possible as shown by the graph composed of a cycle on 4 vertices C_4 and a tree T on $n - 3$ vertices sharing a single vertex.

It is easy to see that $Sz^*(G) = Sz(G) = W(G)$ if G is a tree, which means $m = n - 1$. So, the second conjecture considers graphs with $m \geq n$.

This paper is to give confirmative proofs to the two conjectures. In fact, if G is a bipartite graph, then $Sz^*(G) = Sz(G)$. Therefore, if we give a proof to Conjecture 1.1, then Conjecture 1.2 follows immediately.

2 Main results

In [12], Gutman gave another expression for the Szeged index:

$$Sz(G) = \sum_{e=uv \in E} n_u(e)n_v(e) = \sum_{e=uv \in E} \sum_{\{x,y\} \subseteq V} \mu_{x,y}(e)$$

where $\mu_{x,y}(e)$, interpreted as contribution of the vertex pair x and y to the product $n_u(e)n_v(e)$, is defined as follows:

$$\mu_{x,y}(e) = \begin{cases} 1, & \text{if } \begin{cases} d(x,u) < d(x,v) \text{ and } d(y,v) < d(y,u), \\ \text{or} \\ d(x,v) < d(x,u) \text{ and } d(y,u) < d(y,v), \end{cases} \\ 0, & \text{otherwise.} \end{cases}$$

We first show that for a 2-connected bipartite graph Conjecture 1.1 is true.

Lemma 2.1 *Let G be a 2-connected bipartite graph of order $n \geq 4$. Then*

$$Sz(G) - W(G) \geq 4n - 8$$

with equality if and only if $G = C_4$.

Proof. From above expressions, we know that

$$\begin{aligned} Sz(G) - W(G) &= \sum_{\{x,y\} \subseteq V} \sum_{e \in E} \mu_{x,y}(e) - \sum_{\{x,y\} \subseteq V} d(x,y) \\ &= \sum_{\{x,y\} \subseteq V} \left(\sum_{e \in E} \mu_{x,y}(e) - d(x,y) \right). \end{aligned}$$

Claim: For every pair $x, y \in V$, we have

$$\sum_{e \in E} \mu_{x,y}(e) - d(x,y) \geq 1.$$

In fact, if $xy \in E$, that is $d(x,y) = 1$, then we can find a shortest cycle C containing x and y since G is 2-connected. Then, $G[C]$ has no chord. Since G is bipartite, the length of C is even. There is an edge e' which is the antipodal edge of $e = xy$ in C . It is easy to check that $\mu_{x,y}(e') = \mu_{x,y}(e) = 1$. So the claim is true.

If $d(x,y) \geq 2$, let P_1 be a shortest path from x to y and P_2 be a second shortest path from x to y , that is, $P_2 \neq P_1$ and $|P_2| = \min \{|P| \mid P \text{ is a path from } x \text{ to } y \text{ and } P \neq P_1\}$. Since G is 2-connected, P_2 always exists. If there are more than one path satisfying the condition, we choose P_2 as a one having most common vertices with P_1 .

If $E(P_1) \cap E(P_2) = \emptyset$, let $P_1 \cup P_2 = C$, and then $|E(P_2)| \geq |E(P_1)|$ and all the antipodal edges of P_1 in C makes $\mu_{x,y}(e) = 1$. We also know that $\mu_{x,y}(e) = 1$ for all $e \in E(P_1)$. Hence, $\sum_{e \in E} \mu_{x,y}(e) - d(x, y) \geq d(x, y) > 1$.

If $E(P_1) \cap E(P_2) \neq \emptyset$, then $P_1 \triangle P_2 = C$, where C is a cycle. Let $P'_i = P_i \cap C = x'P_iy'$. It is easy to see that $|E(P'_2)| \geq |E(P'_1)|$, and the shortest path from x (or y) to the vertex v in P'_2 is $xP_2x'(yP_2y')$ together with the shortest path from $x'(y')$ to v in C ; otherwise, contrary to the choice of P_2 . So, all the antipodal edges of P'_1 in C makes $\mu_{x,y}(e) = 1$. We also know that $\mu_{x,y}(e) = 1$ for all $e \in E(P_1)$. Hence, $\sum_{e \in E} \mu_{x,y}(e) = |E(P_1)| + d(x', y') \geq d(x, y) + 1$, which proves the claim.

Now let $C = v_1v_2 \cdots v_pv_1$ be a shortest cycle in G , where p is even and $p \geq 4$. Actually, for every $e \in E(C)$ we have that $\mu_{v_i, v_{\frac{p}{2}+i}}(e) = 1$ for $i = 1, 2, \dots, \frac{p}{2}$. Then $\sum_{e \in E} \mu_{v_i, v_{\frac{p}{2}+i}}(e) = |C| = p$, that is, $\sum_{e \in E} \mu_{v_i, v_{\frac{p}{2}+i}}(e) - d(v_i, v_{\frac{p}{2}+i}) = \frac{p}{2} \geq 2$. Combining with the claim, we have that

$$Sz(G) - W(G) \geq \binom{n}{2} + \frac{p}{2} \left(\frac{p}{2} - 1 \right) \geq \binom{n}{2} + 2 \geq 4n - 8.$$

The last two equalities hold if and only if $p = 4$, $n = 4$ or 5 . If $n = 4, p = 4$, then G is a C_4 . If $n = 5, p = 4$, then G is a $K_{2,3}$, and in this case we can easily calculate that $Sz(G) - W(G) > 12$. Thus, the equality holds if and only if $G = C_4$. ■

Next we will complete the proof of Conjecture 1.1 in general.

Theorem 2.2 *Let G be a bipartite connected graph with $n \geq 4$ vertices and $m \geq n$ edges. Then*

$$Sz(G) - W(G) \geq 4n - 8.$$

Moreover the bound is best possible as shown by the graph composed of a cycle on 4 vertices C_4 and a tree T on $n - 3$ vertices sharing a single vertex.

Proof. We have proved that the conclusion is true for a 2-connected bipartite graph. Now suppose that G is a connected bipartite graph with blocks B_1, B_2, \dots, B_k , where $k \geq 2$. Let $|B_i| = n_i$. Then, $n_1 + n_2 + \dots + n_k = n + k - 1$. Since $m \geq n$ and G is bipartite, there exists at least one block, say B_1 , such that $n_1 \geq 4$. Consider a pair $\{x, y\} \subseteq V$. We have the following observations:

Obs.1: $x, y \in B_i$, and $n_i \geq 4$. For every $e \in B_j, j \neq i, \mu_{x,y}(e) = 0$, combining with Lemma 2.1, we have that

$$\sum_{\{x,y\} \subseteq B_i} \left(\sum_{e \in E} \mu_{x,y}(e) - d(x, y) \right) = \sum_{\{x,y\} \subseteq B_i} \left(\sum_{e \in E(B_i)} \mu_{x,y}(e) - d(x, y) \right) \geq 4n_i - 8.$$

Obs.2: $x, y \in B_i$, and $n_i = 2$. In this case,

$$\sum_{\{x,y\} \subseteq B_i} \left(\sum_{e \in E} \mu_{x,y}(e) - d(x, y) \right) = 0 = 4n_i - 8.$$

Obs.3: $x \in B_1, y \in B_i, i \neq 1$. Let P be a shortest path from x to y , and let w_1, w_i be the cut vertices in B_1 and B_i such that every path from a vertex in B_1 to B_i must go through w_1, w_i . By the proof of Lemma 2.1, we can find an edge $e' \in E(B_1) \setminus E(P)$ such that $\mu_{x,w_1}(e') = 1$. Because every path from a vertex in B_1 to y must go through w_1 , we have $\mu_{x,y}(e') = 1$. We also know that $\mu_{x,y}(e) = 1$ for all $e \in E(P)$. Hence, $\sum_{e \in E} \mu_{x,y}(e) - d(x, y) \geq 1$.

We are now in a position to show that for all $y \in B_i \setminus \{w_i\}$, we can find a vertex $z \in B_1 \setminus \{w_1\}$ such that $\sum_{e \in E} \mu_{z,y}(e) - d(z, y) \geq 2$. Since B_1 is 2-connected with $n_1 \geq 4$, there is a cycle containing w_1 . Let C be a shortest cycle containing w_1 , say $C = v_1 v_2 \cdots v_p v_1$, where $v_1 = w_1$, p is even. Set $z = v_{\frac{p}{2}+1}$. By the proof of Lemma 2.1, we have that $\sum_{e \in E(B_1)} \mu_{z,w_1}(e) - d(z, w_1) \geq \frac{p}{2} \geq 2$. It follows that there are two edges e', e'' which are not in the shortest path from z to w_1 such that $\mu_{z,w_1}(e') = 1, \mu_{z,w_1}(e'') = 1$. Thus, $\mu_{z,y}(e') = 1, \mu_{z,y}(e'') = 1$. Hence, $\sum_{e \in E} \mu_{z,y}(e) - d(z, y) \geq 2$.

If we fix B_i , we obtain that

$$\sum_{\substack{x \in B_1 \setminus \{w_1\} \\ y \in B_i \setminus \{w_i\}}} \left(\sum_{e \in E} \mu_{x,y}(e) - d(x, y) \right) \geq (n_1 - 1)(n_i - 1) + (n_i - 1) = n_1(n_i - 1).$$

Obs.4: $x \in B_i, y \in B_j, i \geq 2, j \geq 2, i \neq j$. Let P be a shortest path between x and y . If P passes through a block B_l with $n_l \geq 4$, and $|B_l \cap P| \geq 2$, then we have that $\sum_{e \in E} \mu_{x,y}(e) - d(x, y) \geq 1$. Otherwise, $\sum_{e \in E} \mu_{x,y}(e) - d(x, y) \geq 0$. So,

$$\sum_{x \in B_i \setminus \{w_i\}, y \in B_j \setminus \{w_j\}} \left(\sum_{e \in E} \mu_{x,y}(e) - d(x, y) \right) \geq 0.$$

Equality holds if and only if P passes through a block B_l with $n_l = 2$ or $n_l \geq 4$, and $|B_l \cap P| = 1$.

From the above observations, we have that

$$\begin{aligned}
& Sz(G) - W(G) \\
&= \sum_{\{x,y\} \subseteq V} \sum_{e \in E} \mu_{x,y}(e) - \sum_{\{x,y\} \subseteq V} d(x,y) \\
&= \sum_{\{x,y\} \subseteq V} \left(\sum_{e \in E} \mu_{x,y}(e) - d(x,y) \right) \\
&= \sum_{i=1}^k \sum_{\{x,y\} \subseteq B_i} \left(\sum_{e \in E} \mu_{x,y}(e) - d(x,y) \right) + \sum_{j=2}^k \sum_{\substack{x \in B_1 \setminus \{w_1\} \\ y \in B_j \setminus \{w_j\}}} \left(\sum_{e \in E} \mu_{x,y}(e) - d(x,y) \right) \\
&\quad + \frac{1}{2} \sum_{\substack{i \neq j \\ i \neq 1, j \neq 1}} \sum_{\substack{x \in B_i \setminus \{w_i\} \\ y \in B_j \setminus \{w_j\}}} \left(\sum_{e \in E} \mu_{x,y}(e) - d(x,y) \right) \\
&\geq \sum_{i=1}^k (4n_i - 8) + n_1 \sum_{j=2}^k (n_j - 1) \\
&= 4(n + k - 1) - 8k + n_1(n - n_1) \\
&= 4n - 4k - 4 + n_1(n - n_1).
\end{aligned}$$

Since $n_1 + n_2 + \cdots + n_k = n + k - 1$, $n_1 \geq 4$, $n_i \geq 2$, for $2 \leq i \leq k$, we have that $4 \leq n_1 \leq n - k + 1$, and $2 \leq k \leq n - 3$.

If $k \geq 5$, then $n_1(n - n_1) \geq 4(n - 4)$. Thus,

$$4n - 4k - 4 + n_1(n - n_1) \geq 8n - 4k - 20 \geq 8n - 4(n - 3) - 20 = 4n - 8.$$

Equality holds if and only if $n_1 = 4$, $n_2 = n_3 = \cdots = n_{n-3} = 2$, and B_2, B_3, \dots, B_{n-3} form a tree T on $n - 3$ vertices, which shares a single vertex with B_1 .

If $2 \leq k \leq 4$, then $n_1(n - n_1) \geq (n - k + 1)(k - 1)$.

If $k = 2$, then $4n - 4k - 4 + (n - k + 1)(k - 1) = 5n - 13 \geq 4n - 8$. Equality holds if and only if $n = 5$, G is a graph composed of a cycle on 4 vertices and a pendant edge.

If $k = 3$, then $4n - 4k - 4 + (n - k + 1)(k - 1) = 6n - 20 \geq 4n - 8$. Equality holds if and only if $n = 6$, G is a graph composed of a cycle on 4 vertices and a tree on 3 vertices sharing a single vertex.

If $k = 4$, then $4n - 4k - 4 + (n - k + 1)(k - 1) = 7n - 29 \geq 4n - 8$. Equality holds if and only if $n = 7$, G is a graph composed of a cycle on 4 vertices and a tree on 4 vertices sharing a single vertex. \blacksquare

Since G is a bipartite graph, $n_0(e) = 0$, and thus $Sz^*(G) = Sz(G)$. So we have the following corollary.

Corollary 2.3 [Conjecture 1.2] *Let G be a bipartite connected graph with $n \geq 4$ vertices and $m \geq n$ edges. Then*

$$Sz^*(G) - W(G) \geq 4n - 8.$$

Moreover the bound is best possible as shown by the graph composed of a cycle on 4 vertices C_4 and a tree T on $n - 3$ vertices sharing a single vertex.

References

- [1] M. Aouchiche, P. Hansen, On a conjecture about the Szeged index, European J. Combin. 31(2010), 1662-1666.
- [2] J.A. Bondy, U.S.R. Murty, *Graph Theory*, GTM 244, Springer, 2008.
- [3] I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, Graph Theory Notes of New York 27(1994), 9-15.
- [4] I. Gutman, S. Klavžar, B. Mohar(Eds), Fifty years of the Wiener index, MATCH Commun. Math. Comput. Chem. 35(1997), 1-259.
- [5] I. Gutman, O.E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, Berlin, 1986.
- [6] I. Gutman, Y.N. Yeh, S.L. Lee, Y.L. Luo, Some recent results in the theory of the Wiener number, Indian J. Chem. 32A(1993), 651-661.
- [7] P. Hansen, Computers and conjectures in chemical graph theory, Plenary speech in the International Conference on Mathematical Chemistry, August 4-7, 2010, Xiamen, China.
- [8] X. Li, M. Liu, Bicyclic graphs with maximal revised Szeged index, arXiv:1104.2122[math.CO], 2011.
- [9] T. Pisanski, M. Randić, Use of the Szeged index and the revised Szeged index for measuring network bipartivity, Discrete Appl. Math. 158(2010), 1936-1944.
- [10] T. Pisanski, J. Žerovnik, Edge-contributions of some topological indices and arboreality of molecular graphs, Ars Math. Contemp. 2(2009), 49-58.
- [11] M. Randić, On generalization of Wiener index for cyclic structures, Acta Chim. Slov. 49(2002), 483-496.
- [12] S. Simić, I. Gutman, V. Baltić, Some graphs with extremal Szeged index, Math. Slovaca 50(2000), 1-15.

- [13] H. Wiener, Structural determination of paraffin boiling points, J. Am. Chem. Soc. 69(1947), 17-20.
- [14] R. Xing, B. Zhou, On the revised Szeged index, Discrete Appl. Math. 159(2011), 69-78.